

Electronic Supplementary Information (ESI)

Solid-state to solution helicity inversion of pseudotetrahedral chiral copper(II) complexes with 2,4-dihalo-salicylaldiminate ligands

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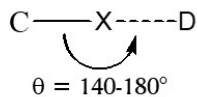
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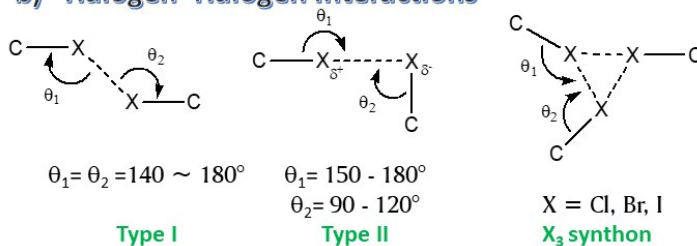
All email addresses: nazanin8821@yahoo.com, h.a.rudbari@sci.ui.ac.ir, gbruno@unime.it, rosario.scopelliti@epfl.ch, braunj37@myumanitoba.ca, david.herbert@umanitoba.ca, olivier.blacque@chem.uzh.ch, icorreia@tecnico.ulisboa.pt, md.aznahid@gmail.com, enamullah@juniv.edu, janiak@uni-duesseldorf.de

a) Halogen Bonding

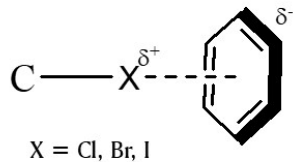


X (acceptor) = Cl, Br, I
Electrophilic species
 (Lewis acid)
 D (donor) = O, N, S, Se
lone pair-possessing species
 (Lewis base)

b) Halogen-Halogen Interactions



c) Halogen- π Interactions



Scheme S1 Schematic representations of three intermolecular halogen interactions: halogen bonds, halogen-halogen interactions and halogen- π interactions.

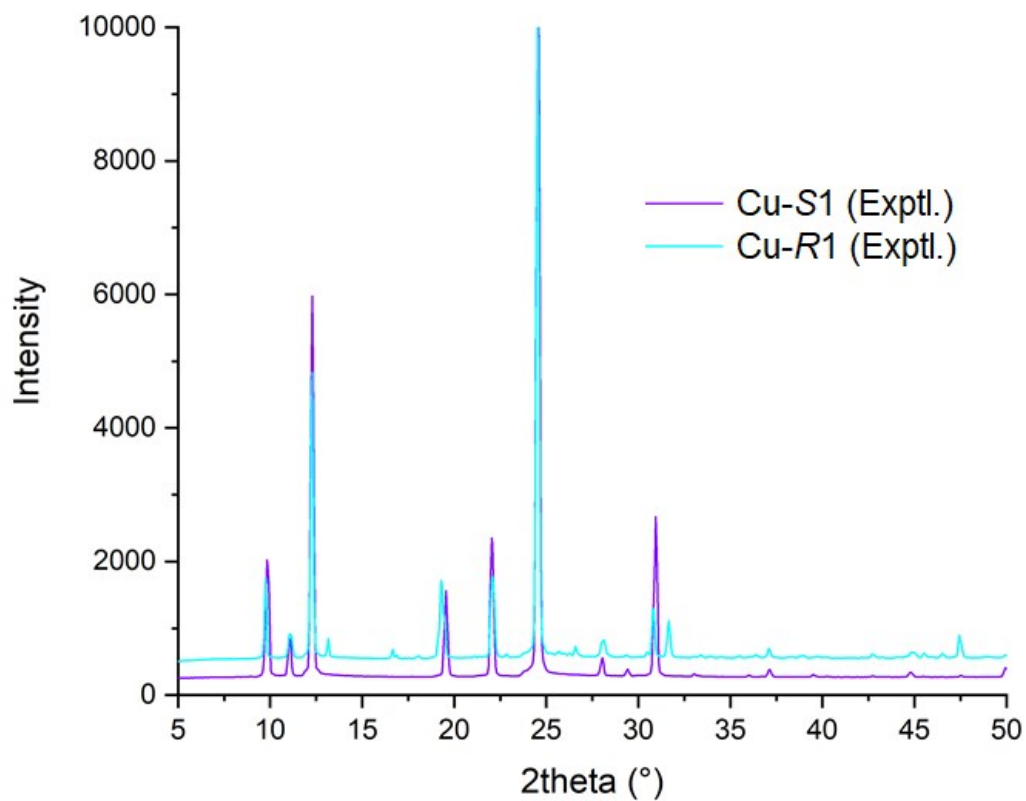


Fig. S1 Experimental PXRD patterns for the bulk samples of Cu-S1 and Cu-R1 at ambient temperature (samples taken from the bulk phase of crystals).

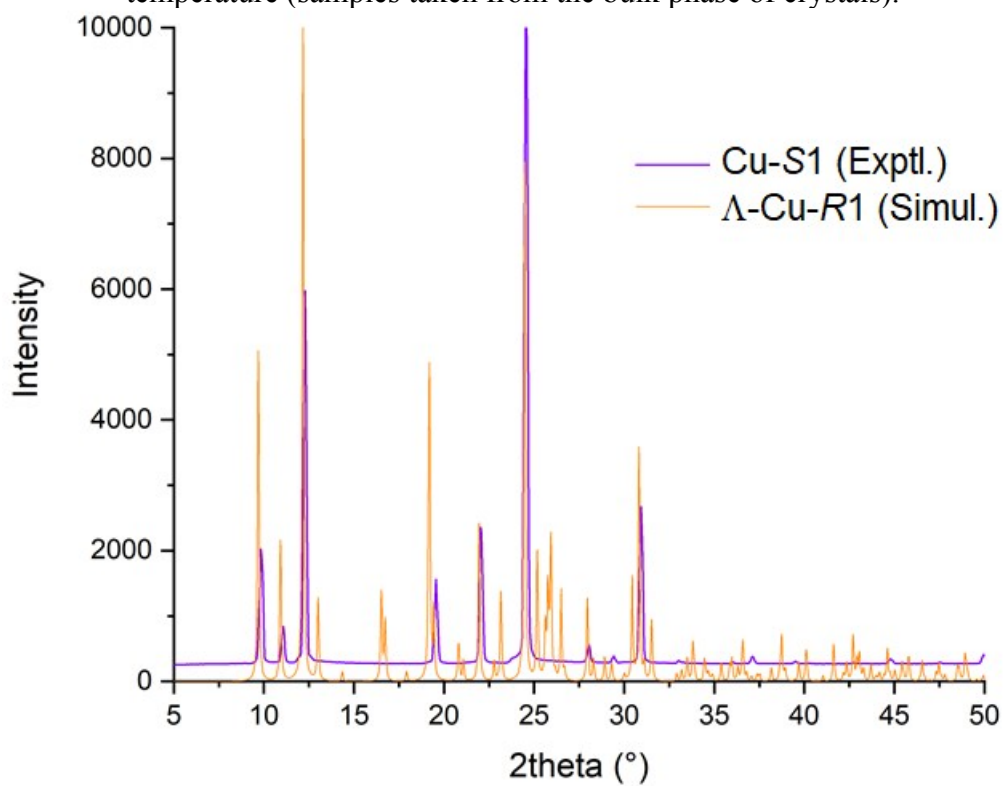


Fig. S2 PXRD for Cu-S1 shows reasonable match to the simulation from the single crystal of Δ -Cu-R1 (samples taken from the bulk phase of Cu-R1).

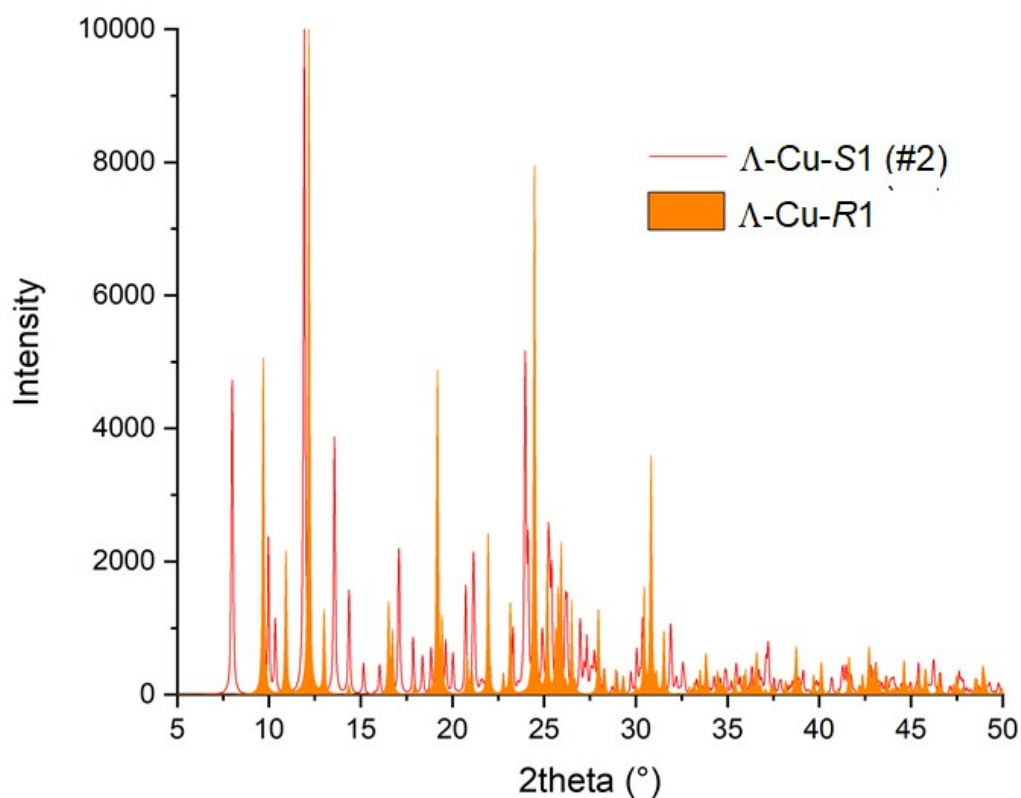


Fig. S3 Simulated PXRD for Λ -Cu-S1 (#2) and Λ -Cu-R1 (for clarity the area under the orange curve for Λ -Cu-R1 has been filled).

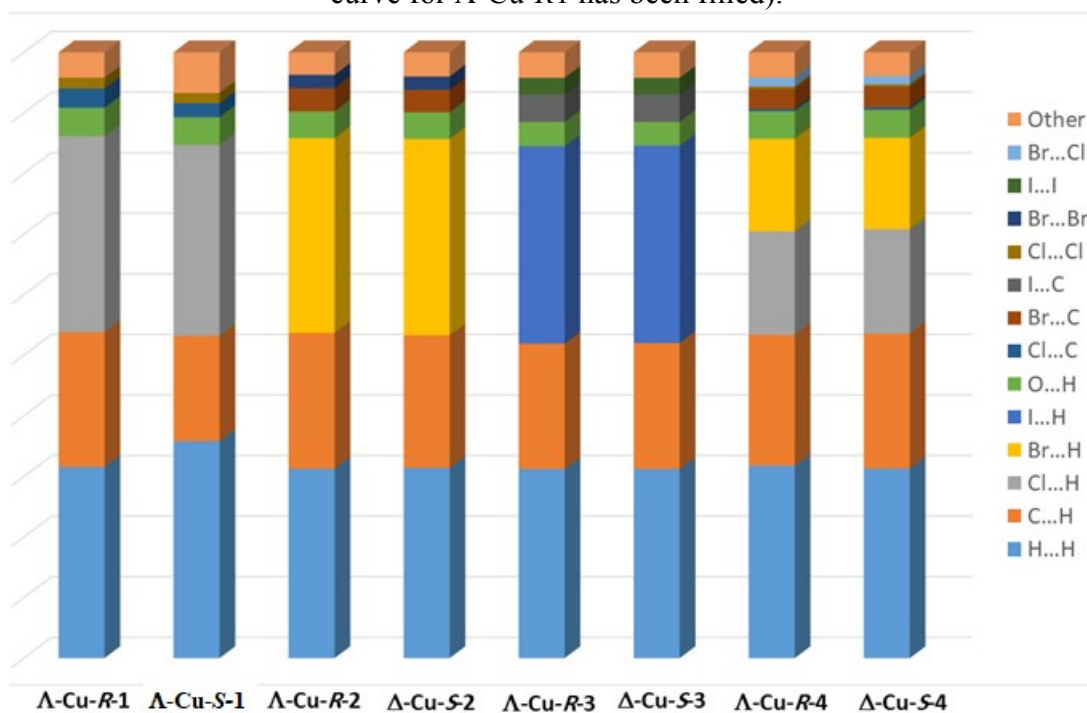


Fig. S4 Relative contributions to the Hirshfeld surfaces area for different intermolecular contacts in the complexes.

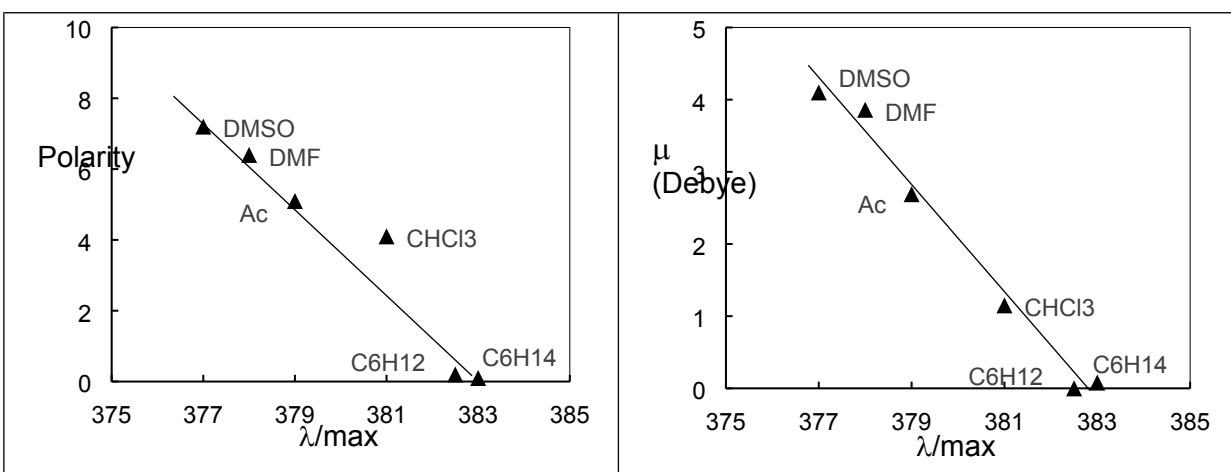
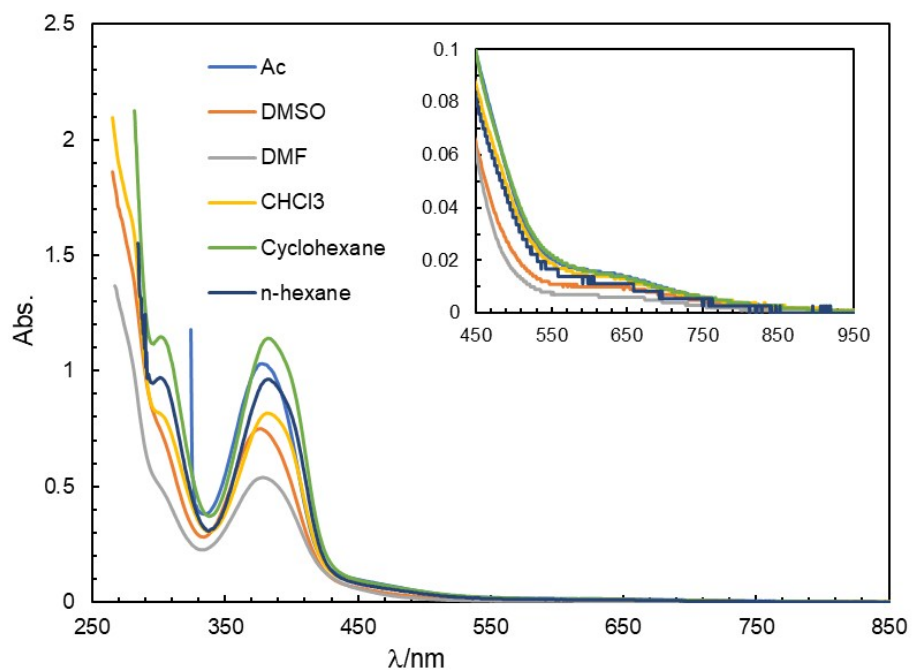
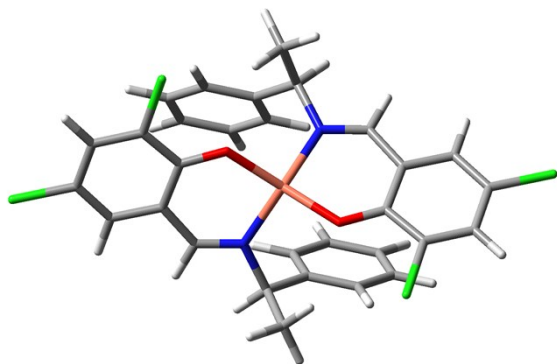
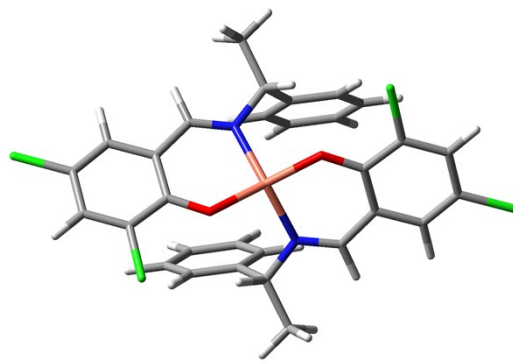


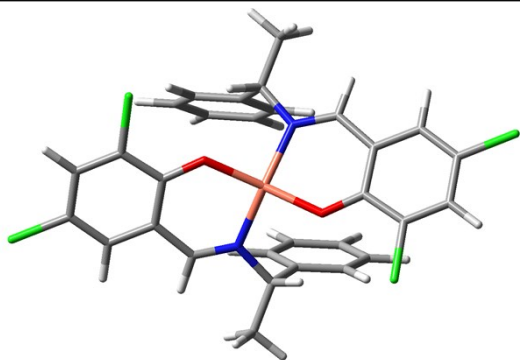
Fig. S5 (a) UV-Vis. spectra for Cu-R2 in different solvents at 25 °C (top); (b) Changes of absorption maxima (λ /max) of MLCT bands in the solvents of increasing polarity (P) and dipole moment (μ /Debye) (bottom).



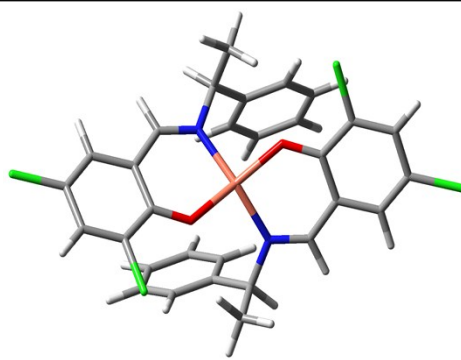
Λ -Cu-R1 (−4898.371829 a.u.)



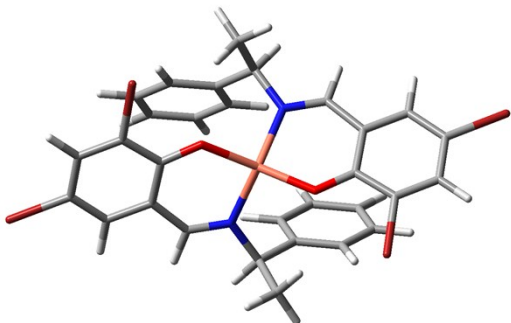
Δ -Cu-R1 (−4898.376386 a.u.), (stable by −2.86 Kcal/mol)



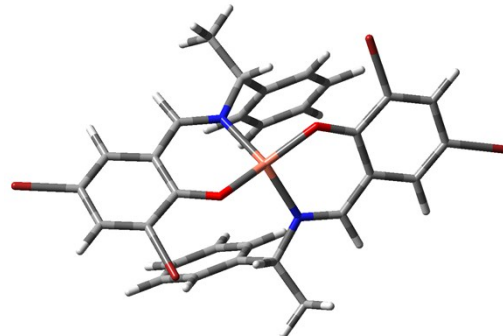
Λ -Cu-S1 (#1) (−4898.380224 a.u.), (stable by −4.57 Kcal/mol)



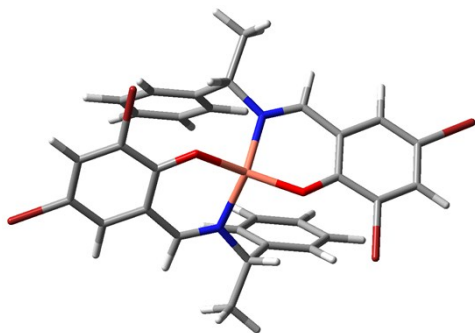
Δ -Cu-S1 (#1) (−4898.372945 a.u.)



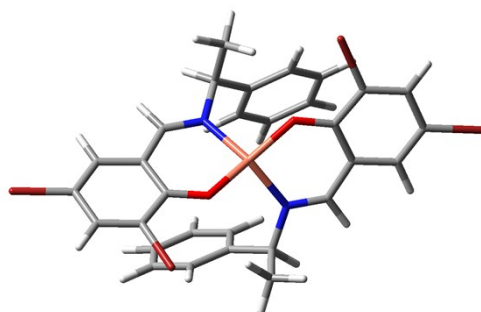
Λ -Cu-R2 (−13344.420635 a.u.)



Δ -Cu-R2 (−13344.422295 a.u.), (stable by −1.04 Kcal/mol)



Λ -Cu-S2 (−13344.422334 a.u.), (stable by −0.96 Kcal/mol)



Δ -Cu-S2 (−13344.420798 a.u.)

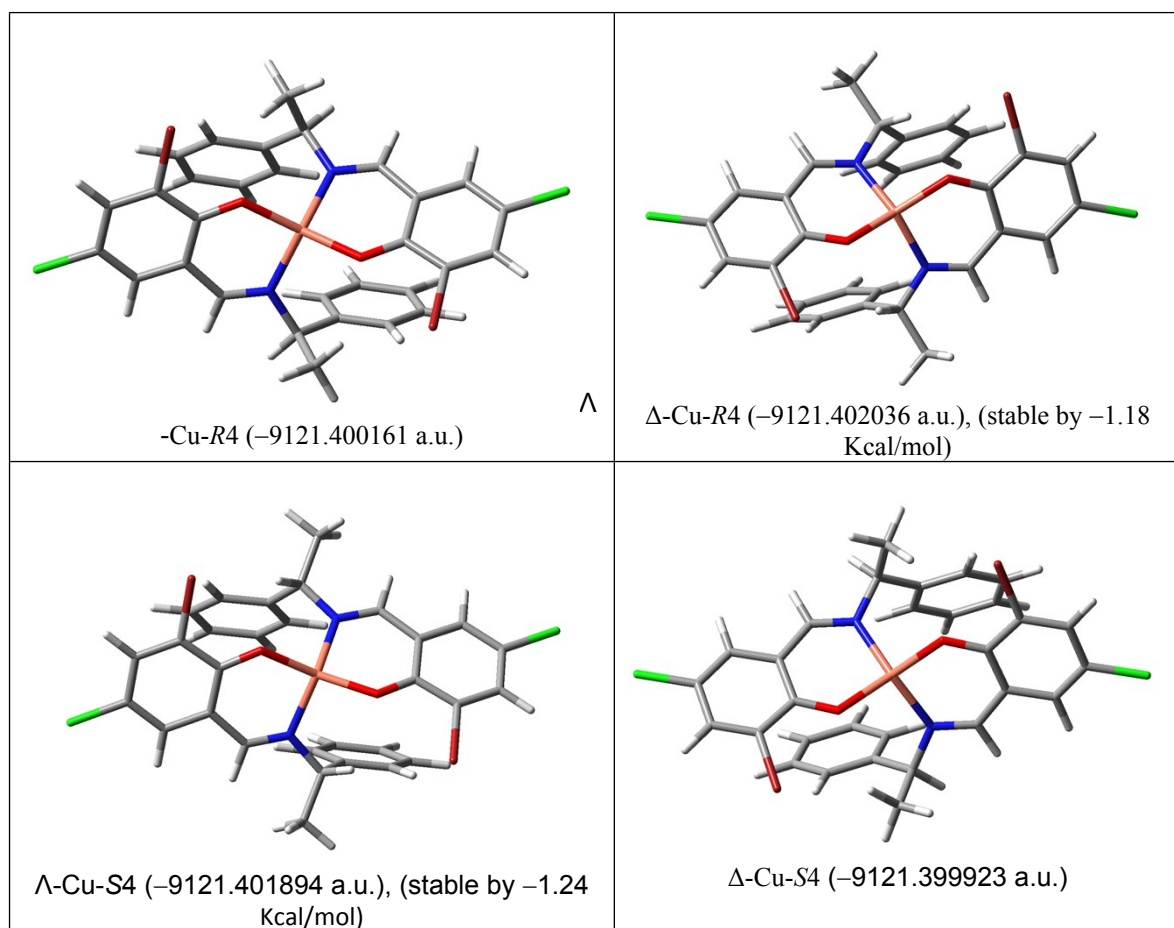


Fig. S6 DFT-optimized structures for diastereomeric pairs Λ -Cu-R2/ Δ -Cu-R2, Λ -Cu-S2/ Δ -Cu-S2, Λ -Cu-R4/ Δ -Cu-R4 and Λ -Cu-S4/ Δ -Cu-S4 at b3lyp/6-31G(d), respectively.

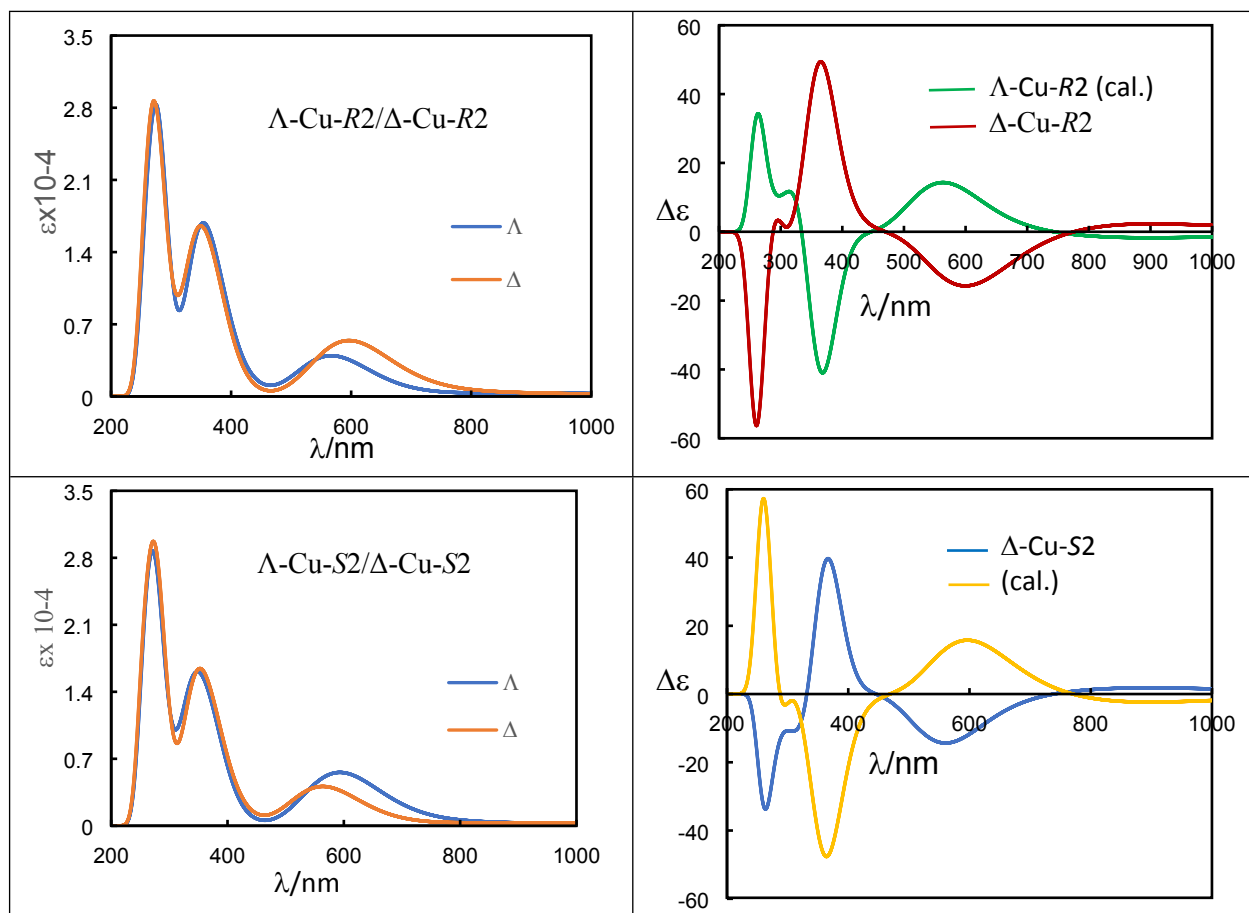


Fig. S7 Simulated UV-Vis. and ECD spectra for the diastereomeric pairs Δ -Cu-R2/ Δ -Cu-R2 and Δ -Cu-S2/ Δ -Cu-S2 at m06/tzvp//b3lyp/6-31G(d), (Gaussian band shape with exponential half-width $\sigma = 0.33$ eV).

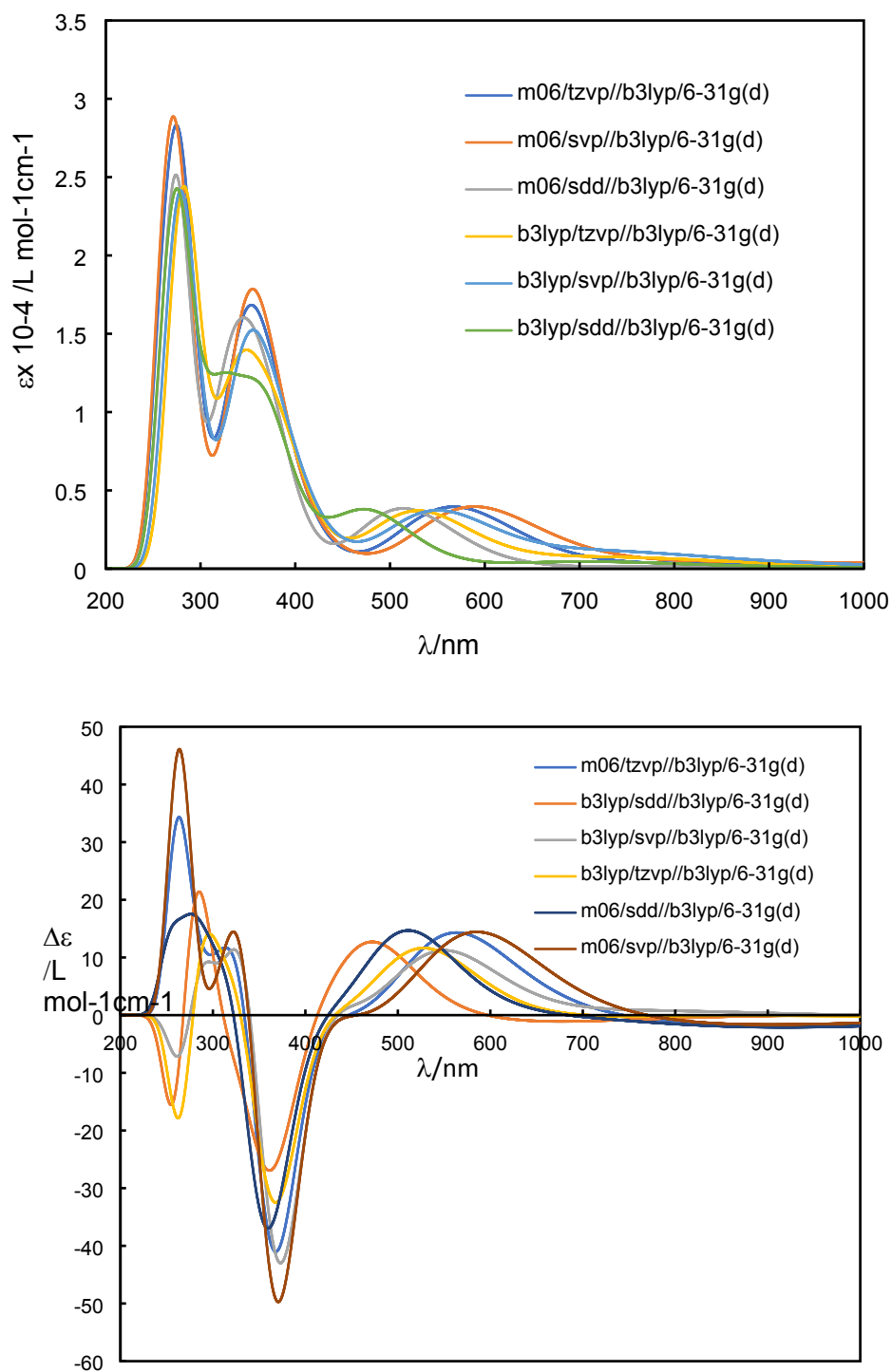


Fig. S8 Simulated UV-Vis. (top) and ECD (bottom) spectra for the Λ -Cu-R2 with different combinations of the functionals and the basis sets (Gaussian band shape with exponential half-width $\sigma = 0.33$ eV).

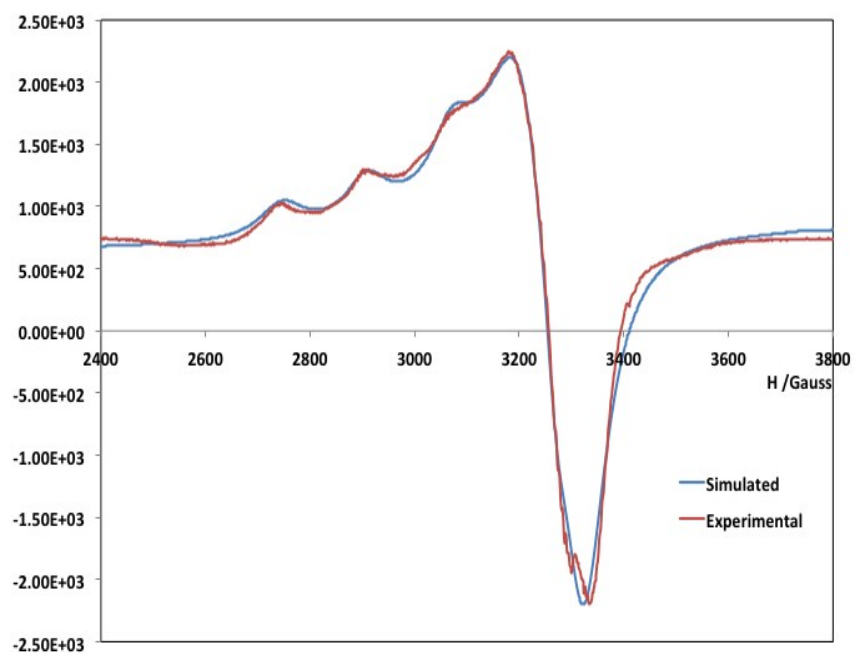


Fig. S9 Experimental and simulated spectra for Cu-S1 measured in CH_2Cl_2 (*ca.* 3.0 mM) at *ca.* 100 K.

Table S1 Excited states, MOs contributions, excitation energy (eV), wavelength (nm) and oscillator strength (f) for Δ -CuR2 at m06/tzvp//b3lyp/631g(d) in chloroform.

Excited State 1: 2.006-A 0.8694 eV 1426.05 nm f=0.0010 $\langle S^2 \rangle = 0.756$

165B ->202B	-0.14276
168B ->202B	-0.16259
171B ->202B	-0.14559
172B ->202B	0.12946
175B ->202B	-0.22234
180B ->202B	-0.31083
183B ->202B	-0.15783
191B ->202B	-0.12503
193B ->202B	-0.52340
196B ->202B	0.30126
197B ->202B	0.16378
199B ->202B	-0.11679
201B ->202B	0.56559

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-KS) = -13353.7873580

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: 2.007-A 1.3350 eV 928.71 nm f=0.0000 $\langle S^2 \rangle = 0.757$

164B ->202B	0.16893
166B ->202B	-0.25246
173B ->202B	-0.25807
174B ->202B	0.15198
176B ->202B	-0.34989
178B ->202B	-0.23542
181B ->202B	0.12795
185B ->202B	-0.45684
189B ->202B	0.14994
192B ->202B	0.28953
200B ->202B	0.51152

Excited State 3: 2.004-A 1.4241 eV 870.62 nm f=0.0057 $\langle S^2 \rangle = 0.754$

169B ->202B	0.14801
171B ->202B	0.23370
175B ->202B	0.19266
177B ->202B	0.13975
180B ->202B	-0.47055
183B ->202B	-0.22811
186B ->202B	0.62031

188B ->202B	-0.16408
190B ->202B	0.12788
193B ->202B	0.20360
196B ->202B	-0.16876
199B ->202B	0.10359
201B ->202B	0.20315

Excited State 4: 2.003-A 1.5962 eV 776.76 nm f=0.0005 $\langle S^{*2} \rangle = 0.753$

160B ->202B	-0.12414
164B ->202B	0.21173
173B ->202B	-0.11911
174B ->202B	0.20854
176B ->202B	0.33260
178B ->202B	0.11655
181B ->202B	0.20323
182B ->202B	0.33066
184B ->202B	0.68465
189B ->202B	0.11502
192B ->202B	0.15235
195B ->202B	-0.18740
200B ->202B	-0.17725

Excited State 5: 2.037-A 2.0797 eV 596.16 nm f=0.1101 $\langle S^{*2} \rangle = 0.787$

165B ->202B	0.12732
168B ->202B	0.12491
180B ->202B	0.34689
183B ->202B	0.11724
186B ->202B	-0.14575
193B ->202B	0.35424
196B ->202B	-0.12458
201B ->202B	0.78444

Excited State 6: 2.040-A 2.2228 eV 557.79 nm f=0.0003 $\langle S^{*2} \rangle = 0.790$

166B ->202B	0.20971
173B ->202B	0.11150
176B ->202B	0.30083
178B ->202B	0.18567
185B ->202B	0.26567
195B ->202B	-0.11285
200B ->202B	0.81648

Excited State 7: 3.402-A 2.6499 eV 467.89 nm f=0.0000 $\langle S^{*2} \rangle = 2.644$

201A ->204A	-0.48519
202A ->203A	-0.49922
200B ->204B	-0.39163
201B ->203B	0.53470

Excited State 8: 3.396-A 2.6507 eV 467.74 nm f=0.0006 <S**2>=2.634

201A ->203A	-0.49532
202A ->204A	-0.49800
200B ->203B	-0.39451
201B ->204B	0.52266

Excited State 9: 2.143-A 3.0126 eV 411.55 nm f=0.0074 <S**2>=0.898

196B ->202B	0.32845
199B ->202B	0.89637

Excited State 10: 2.249-A 3.0324 eV 408.86 nm f=0.0002 <S**2>=1.015

196A ->203A	0.11767
195B ->202B	0.14365
196B ->203B	-0.11561
198B ->202B	0.91178

Excited State 11: 3.348-A 3.1077 eV 398.96 nm f=0.0012 <S**2>=2.553

194A ->203A	0.16570
195A ->203A	0.15712
196A ->204A	0.32489
197A ->203A	-0.10390
199A ->204A	0.15143
200A ->203A	0.30022
201A ->207A	-0.17766
201A ->210A	0.10710
202A ->208A	-0.15118
202A ->211A	0.15880
193B ->202B	0.10110
194B ->203B	0.10686
195B ->203B	-0.24155
196B ->204B	-0.31498
198B ->203B	-0.23337
199B ->202B	-0.23710
199B ->204B	-0.14462
200B ->203B	-0.19383
200B ->207B	-0.16216
200B ->210B	0.12769

201B ->204B	0.11106
201B ->208B	0.14202
201B ->211B	-0.17235

Excited State 12: 3.288-A 3.1146 eV 398.07 nm f=0.0000 <S**2>=2.453

194A ->204A	-0.16002
195A ->204A	-0.15227
196A ->203A	-0.31870
197A ->204A	0.10018
199A ->203A	-0.14954
200A ->204A	-0.28875
201A ->208A	0.14331
201A ->211A	-0.14915
202A ->207A	0.17028
202A ->210A	-0.10297
194B ->204B	-0.10301
195B ->204B	0.23420
196B ->203B	0.31247
198B ->202B	0.33546
198B ->204B	0.22683
199B ->203B	0.14431
200B ->204B	0.18617
200B ->208B	0.13006
200B ->211B	-0.15959
201B ->207B	-0.16810
201B ->210B	0.13079

Excited State 13: 2.028-A 3.2303 eV 383.81 nm f=0.0002 <S**2>=0.779

196B ->202B	-0.30141
197B ->202B	0.93909

Excited State 14: 2.074-A 3.2599 eV 380.33 nm f=0.0182 <S**2>=0.825

190B ->202B	0.11115
193B ->202B	0.48360
196B ->202B	0.74887
197B ->202B	0.23501
199B ->202B	-0.27583

Excited State 15: 2.055-A 3.3022 eV 375.46 nm f=0.0074 <S**2>=0.805

201A ->204A	-0.18905
202A ->203A	-0.14056
184B ->202B	0.13310

194B ->202B	-0.18135
195B ->202B	0.84177
198B ->202B	-0.17656
200B ->204B	0.15849
201B ->203B	-0.27023

Excited State 16: 2.087-A 3.3339 eV 371.89 nm f=0.1073 <S**2>=0.839

201A ->203A	0.46163
202A ->204A	0.37008
180B ->202B	-0.20598
183B ->202B	-0.16751
186B ->202B	-0.23308
188B ->202B	0.10698
191B ->202B	-0.15674
193B ->202B	0.21620
197B ->202B	-0.10751
199B ->202B	0.10797
200B ->203B	-0.27993
201B ->204B	0.53768

Excited State 17: 2.086-A 3.3646 eV 368.50 nm f=0.0422 <S**2>=0.838

201A ->204A	0.47964
202A ->203A	0.40954
195B ->202B	0.39472
200B ->204B	-0.25157
201B ->203B	0.57515

Excited State 18: 2.169-A 3.4394 eV 360.48 nm f=0.0005 <S**2>=0.926

194B ->202B	0.93296
195B ->202B	0.20942

Excited State 19: 3.458-A 3.4603 eV 358.30 nm f=0.0001 <S**2>=2.739

194A ->209A	0.10135
194A ->210A	-0.11413
195A ->209A	-0.14646
195A ->210A	0.12259
195A ->212A	-0.14188
197A ->210A	0.18935
197A ->212A	0.18429
198A ->206A	0.30940
198A ->208A	-0.13007
199A ->205A	0.35408

200A ->210A	0.13515
200A ->212A	0.15746
194B ->207B	-0.11055
194B ->209B	0.21819
194B ->210B	-0.12912
195B ->212B	0.17884
197B ->206B	0.30329
198B ->210B	-0.19481
198B ->212B	-0.20515
199B ->205B	-0.33925

Excited State 20: 3.374-A 3.4862 eV 355.64 nm f=0.0000 <S**2>=2.596

194A ->206A	-0.13073
195A ->206A	0.21715
197A ->205A	0.25554
198A ->207A	0.10780
198A ->209A	-0.17116
198A ->212A	-0.22668
199A ->210A	0.26329
199A ->212A	0.16943
200A ->205A	0.18981
200A ->206A	-0.10178
194B ->202B	0.27131
194B ->205B	-0.19888
194B ->206B	0.18407
195B ->206B	0.19116
197B ->207B	-0.11448
197B ->209B	0.20175
197B ->212B	0.20323
198B ->205B	-0.26701
198B ->206B	-0.14191
199B ->209B	0.12805
199B ->210B	-0.22455
199B ->212B	-0.18103

Excited State 21: 2.572-A 3.5956 eV 344.82 nm f=0.0178 <S**2>=1.403

193A ->204A	0.16757
194A ->203A	-0.12884
197A ->203A	-0.15055
200A ->203A	0.23534
201A ->203A	0.63687
202A ->204A	-0.54950

180B ->202B	0.14059
186B ->202B	0.14627
191B ->202B	0.13218
193B ->202B	-0.13690
196B ->202B	0.14150

Excited State 22: 2.545-A 3.5988 eV 344.52 nm f=0.0005 <S**2>=1.369

193A ->203A	-0.17204
194A ->204A	0.13355
197A ->204A	0.15913
200A ->204A	-0.25713
201A ->204A	-0.60205
202A ->203A	0.66994

Excited State 23: 2.052-A 3.6535 eV 339.36 nm f=0.2108 <S**2>=0.803

202A ->204A	0.43837
165B ->202B	0.13826
168B ->202B	0.13093
175B ->202B	0.18224
180B ->202B	0.30553
183B ->202B	0.16979
186B ->202B	0.32356
188B ->202B	-0.15703
191B ->202B	0.29428
193B ->202B	-0.36922
196B ->202B	0.24026
201B ->204B	0.34149

Excited State 24: 3.058-A 3.7388 eV 331.61 nm f=0.0063 <S**2>=2.087

201A ->207A	-0.16173
202A ->204A	-0.11591
202A ->208A	-0.14739
202A ->211A	0.12617
200B ->203B	0.74381
200B ->207B	-0.15206
200B ->210B	0.10189
201B ->204B	0.46297
201B ->208B	0.12638
201B ->211B	-0.11655

Excited State 25: 3.098-A 3.7472 eV 330.87 nm f=0.0023 <S**2>=2.150

201A ->208A	-0.15455
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201A ->211A	0.13542
202A ->203A	-0.12711
202A ->207A	-0.17268
200B ->204B	0.73850
200B ->208B	-0.13565
200B ->211B	0.14882
201B ->203B	0.44419
201B ->207B	0.14383

Excited State 26: 3.212-A 3.8070 eV 325.67 nm f=0.0008 <S**2>=2.329

194A ->204A	0.10202
196A ->203A	0.20391
199A ->203A	0.11846
200A ->204A	0.21746
201A ->204A	-0.11934
201A ->206A	0.11256
201A ->208A	0.24143
201A ->211A	-0.20526
202A ->207A	0.27436
202A ->210A	-0.13661
202A ->212A	0.11734
195B ->204B	-0.15800
196B ->203B	-0.17852
198B ->204B	-0.17408
200B ->204B	0.38190
200B ->208B	0.21138
200B ->211B	-0.20639
201B ->203B	0.25669
201B ->207B	-0.30253
201B ->210B	0.19325
201B ->212B	-0.13520

Excited State 27: 3.203-A 3.8081 eV 325.58 nm f=0.0055 <S**2>=2.314

194A ->203A	0.10025
196A ->204A	0.20162
199A ->204A	0.11799
200A ->203A	0.24179
201A ->203A	-0.13477
201A ->207A	0.26860
201A ->210A	-0.13664
201A ->212A	0.11222
202A ->206A	0.11028

202A ->208A	0.24429
202A ->211A	-0.20459
195B ->203B	-0.15521
196B ->204B	-0.15953
198B ->203B	-0.16905
200B ->203B	0.35772
200B ->207B	0.24442
200B ->210B	-0.15704
200B ->212B	0.12250
201B ->204B	0.21677
201B ->206B	0.11693
201B ->208B	-0.26047
201B ->211B	0.26612

Excited State 28: 2.705-A 4.0543 eV 305.81 nm f=0.0011 <S**2>=1.579

190A ->203A	0.10127
193A ->203A	0.20968
194A ->204A	-0.27393
195A ->204A	-0.19552
196A ->203A	-0.12822
197A ->204A	-0.28000
199A ->203A	0.13260
200A ->204A	0.53533
201A ->204A	-0.28668
202A ->203A	0.22037
192B ->202B	0.31257
193B ->203B	-0.10305
195B ->204B	0.11095
196B ->203B	0.20434

Excited State 29: 2.809-A 4.0577 eV 305.56 nm f=0.0283 <S**2>=1.722

190A ->204A	0.11301
193A ->204A	0.23823
194A ->203A	-0.31860
195A ->203A	-0.22736
196A ->204A	-0.16713
197A ->203A	-0.29459
199A ->204A	0.14209
200A ->203A	0.57989
201A ->203A	-0.28306
202A ->204A	0.26491
195B ->203B	0.11654

196B ->204B 0.19216

Excited State 30: 2.143-A 4.0862 eV 303.42 nm f=0.0012 <S**2>=0.899

193A ->203A -0.11486

194A ->204A 0.15937

195A ->204A 0.11687

196A ->203A 0.11485

197A ->204A 0.11090

200A ->204A -0.22779

202A ->203A -0.13436

164B ->202B -0.14783

166B ->202B 0.15736

173B ->202B 0.12687

174B ->202B -0.11015

176B ->202B 0.12800

178B ->202B 0.12192

181B ->202B -0.13126

182B ->202B -0.13278

187B ->202B 0.12539

192B ->202B 0.79935

Excited State 31: 3.174-A 4.2170 eV 294.01 nm f=0.0007 <S**2>=2.269

201A ->207A -0.24971

201A ->209A -0.32212

201A ->210A -0.10622

202A ->208A -0.30006

202A ->211A -0.31003

183B ->202B -0.12472

190B ->202B -0.18169

191B ->202B 0.38159

200B ->207B -0.20922

200B ->209B -0.23559

200B ->210B -0.17669

201B ->208B 0.31212

201B ->211B 0.29385

Excited State 32: 2.337-A 4.2179 eV 293.95 nm f=0.0130 <S**2>=1.115

201A ->209A 0.16107

202A ->208A 0.10021

202A ->211A 0.17357

180B ->202B -0.13727

183B ->202B -0.19857

186B ->202B	-0.22881
190B ->202B	0.12826
191B ->202B	0.81049
200B ->209B	0.11184
201B ->208B	-0.14512
201B ->211B	-0.14260

Excited State 33: 3.431-A 4.2184 eV 293.91 nm f=0.0000 <S**2>=2.694

201A ->208A	0.30900
201A ->211A	0.36252
202A ->207A	0.25991
202A ->209A	0.38418
202A ->210A	0.13991
202A ->212A	-0.11274
200B ->208B	0.29598
200B ->211B	0.29628
201B ->207B	-0.27125
201B ->209B	-0.31359
201B ->210B	-0.24488
201B ->212B	0.11905

Excited State 34: 2.163-A 4.2236 eV 293.55 nm f=0.0243 <S**2>=0.920

202A ->211A	-0.10934
171B ->202B	-0.10714
175B ->202B	-0.15731
188B ->202B	-0.18753
190B ->202B	0.88630
201B ->211B	0.11995

Excited State 35: 2.777-A 4.2798 eV 289.70 nm f=0.0026 <S**2>=1.678

200A ->204A	0.17830
185B ->202B	0.18197
189B ->202B	-0.12137
192B ->202B	0.16061
193B ->203B	0.53684
196B ->203B	-0.29110
197B ->203B	-0.26834
199B ->203B	0.58132

Excited State 36: 2.860-A 4.2938 eV 288.75 nm f=0.0071 <S**2>=1.795

200A ->203A	0.18642
193B ->204B	0.56795

196B ->204B	-0.30640
197B ->204B	-0.27947
198B ->203B	0.11873
199B ->204B	0.58037

Excited State 37: 2.139-A 4.3171 eV 287.19 nm f=0.0008 <S**2>=0.894

166B ->202B	0.10023
181B ->202B	-0.16131
182B ->202B	-0.14703
185B ->202B	-0.22248
187B ->202B	-0.34329
189B ->202B	0.80002
199B ->203B	0.19065

Excited State 38: 2.365-A 4.3739 eV 283.46 nm f=0.0001 <S**2>=1.149

196A ->203A	-0.19666
199A ->203A	0.18784
200A ->204A	-0.12111
173B ->202B	-0.12176
176B ->202B	-0.16190
178B ->202B	-0.13441
184B ->202B	-0.12992
185B ->202B	0.55610
187B ->202B	-0.37441
189B ->202B	0.22330
192B ->202B	0.30599
198B ->204B	-0.15266
199B ->203B	-0.23869

Excited State 39: 3.428-A 4.3845 eV 282.78 nm f=0.0016 <S**2>=2.688

193A ->204A	-0.16493
195A ->210A	-0.11318
196A ->204A	-0.11870
197A ->203A	0.36286
197A ->212A	0.11965
198A ->205A	-0.19388
199A ->204A	0.26536
199A ->206A	-0.23942
200A ->212A	0.10192
193B ->204B	0.23881
194B ->203B	-0.14506
194B ->209B	-0.14759

195B ->203B	0.19066
197B ->205B	0.19910
198B ->203B	-0.31155
198B ->212B	-0.13263
199B ->204B	-0.14433
199B ->206B	-0.23588

Excited State 40: 3.261-A 4.3946 eV 282.13 nm f=0.0004 <S**2>=2.409

193A ->203A	-0.16717
195A ->206A	-0.16521
196A ->203A	-0.10319
197A ->204A	0.23494
197A ->205A	0.11348
198A ->203A	0.17471
198A ->209A	0.11693
198A ->210A	-0.10656
199A ->203A	0.42648
199A ->212A	0.13958
200A ->205A	0.11258
185B ->202B	-0.25627
187B ->202B	0.10470
193B ->203B	0.25363
194B ->204B	-0.12475
194B ->206B	-0.16778
195B ->204B	0.13692
197B ->203B	-0.22263
197B ->209B	-0.14986
198B ->205B	-0.13442
199B ->203B	-0.12878
199B ->212B	-0.12807

Excited State 41: 2.866-A 4.4286 eV 279.96 nm f=0.1034 <S**2>=1.804

195A ->203A	0.22727
195A ->212A	0.12509
196A ->204A	0.15500
197A ->210A	0.11617
198A ->204A	0.23307
198A ->205A	0.10691
198A ->206A	-0.19472
199A ->204A	0.19127
199A ->205A	0.20540
200A ->210A	0.10233

202A ->208A	-0.10419
168B ->202B	0.13090
171B ->202B	0.15750
175B ->202B	0.20435
186B ->202B	-0.14939
188B ->202B	0.12614
190B ->202B	0.14729
193B ->202B	-0.14887
194B ->203B	-0.15210
194B ->210B	-0.10118
194B ->212B	-0.11587
195B ->212B	-0.10020
196B ->204B	0.22391
197B ->206B	-0.19478
198B ->203B	0.28749
198B ->209B	0.14281
199B ->205B	-0.19698

Excited State 42: 2.824-A 4.4313 eV 279.79 nm f=0.0921 <S**2>=1.743

193A ->204A	-0.12239
194A ->203A	0.21628
195A ->212A	-0.14157
196A ->204A	0.26362
197A ->203A	0.11340
197A ->210A	-0.12393
198A ->206A	0.20442
199A ->204A	-0.15867
199A ->205A	-0.20292
200A ->203A	0.17551
168B ->202B	0.13295
171B ->202B	0.15864
175B ->202B	0.21120
186B ->202B	-0.14938
188B ->202B	0.12918
190B ->202B	0.15158
193B ->202B	-0.15076
194B ->212B	0.14324
195B ->203B	0.17709
196B ->204B	0.14835
197B ->204B	0.22606
197B ->206B	0.21440
198B ->203B	0.16250

198B ->209B	-0.12923
198B ->210B	0.11019
199B ->205B	0.21116
201B ->208B	-0.13022

Excited State 43: 3.328-A 4.4395 eV 279.28 nm f=0.0006 <S**2>=2.519

194A ->205A	-0.11494
195A ->205A	0.13345
195A ->206A	-0.11417
197A ->204A	-0.11608
197A ->205A	0.15714
197A ->206A	0.16023
198A ->203A	0.37453
198A ->212A	0.20088
199A ->203A	-0.25952
199A ->207A	0.10803
199A ->209A	-0.14909
199A ->210A	0.22057
200A ->205A	0.11309
200A ->206A	0.15992
185B ->202B	0.11182
193B ->203B	-0.14768
194B ->205B	-0.19562
195B ->206B	-0.15114
197B ->203B	-0.27134
197B ->210B	-0.10753
197B ->212B	-0.19663
198B ->205B	-0.19278
198B ->206B	0.17448
199B ->203B	-0.10913
199B ->207B	-0.10378
199B ->209B	0.20786
199B ->210B	-0.15638

Excited State 44: 2.712-A 4.4604 eV 277.97 nm f=0.0112 <S**2>=1.589

193A ->203A	0.17106
194A ->204A	0.13349
195A ->204A	0.12670
197A ->204A	-0.11602
199A ->203A	0.67630
200A ->204A	-0.19457
193B ->203B	-0.20656

198B ->204B	0.30379
199B ->203B	0.30127
201B ->207B	-0.11696

Excited State 45: 2.677-A 4.4768 eV 276.95 nm f=0.0134 <S**2>=1.541

193A ->204A	0.13649
198A ->204A	-0.21410
199A ->204A	0.82116
200A ->203A	-0.29610
198B ->203B	0.12959
199B ->204B	0.18575

Excited State 46: 2.067-A 4.4870 eV 276.32 nm f=0.0002 <S**2>=0.818

196A ->203A	-0.10293
197A ->204A	-0.12293
199A ->203A	0.11522
200A ->204A	-0.13249
201A ->206A	0.10505
201A ->208A	0.35367
201A ->211A	0.22368
202A ->207A	0.33565
202A ->209A	0.27710
200B ->208B	-0.36200
200B ->211B	-0.19827
201B ->207B	0.39433
201B ->209B	0.29253
201B ->210B	0.16631

Excited State 47: 2.046-A 4.4903 eV 276.12 nm f=0.0255 <S**2>=0.797

199A ->204A	0.12729
201A ->207A	0.30045
201A ->209A	0.31282
202A ->208A	0.35373
202A ->211A	0.28366
198B ->203B	0.10394
200B ->207B	-0.29248
200B ->209B	-0.25918
200B ->210B	-0.16533
201B ->205B	0.11458
201B ->208B	0.44320
201B ->211B	0.28801

Excited State 48: 2.133-A 4.5167 eV 274.50 nm f=0.0221 <S**2>=0.887

193A ->203A	-0.18815
194A ->204A	0.16056
195A ->204A	0.12837
196A ->203A	0.21525
197A ->204A	0.40196
198A ->203A	0.24756
200A ->204A	0.39432
201A ->211A	0.15811
202A ->209A	0.15803
176B ->202B	-0.12028
185B ->202B	0.21317
196B ->203B	0.21881
197B ->203B	0.22786
198B ->204B	0.34849
200B ->211B	-0.13692
201B ->209B	0.12900
201B ->210B	0.13200

Excited State 49: 3.210-A 4.5168 eV 274.49 nm f=0.0684 <S**2>=2.325

193A ->204A	0.10842
194A ->203A	0.12625
195A ->210A	-0.13436
196A ->204A	0.10462
197A ->203A	0.13709
197A ->212A	0.12609
198A ->205A	-0.20535
198A ->206A	-0.10156
199A ->205A	0.12407
199A ->206A	-0.14685
200A ->203A	0.19797
200A ->212A	0.11433
191B ->204B	-0.10258
193B ->204B	-0.19787
194B ->209B	-0.13135
195B ->210B	0.12199
197B ->204B	0.11759
197B ->205B	0.23039
198B ->203B	0.21195
198B ->212B	-0.14206
199B ->204B	0.37422
199B ->205B	-0.10783

199B ->206B -0.12647

Excited State 50: 3.225-A 4.5475 eV 272.64 nm f=0.0000 <S**2>=2.350

193A ->203A -0.11908
194A ->206A -0.10241
195A ->205A 0.18584
197A ->205A -0.13434
197A ->206A 0.12890
198A ->203A 0.15315
198A ->209A -0.11349
198A ->210A 0.23685
199A ->203A 0.31998
199A ->212A -0.19629
200A ->205A -0.13354
194B ->204B -0.10721
194B ->205B -0.14575
194B ->206B 0.15624
195B ->205B -0.16823
196B ->203B 0.10590
197B ->209B 0.17691
197B ->210B -0.16231
198B ->204B -0.29676
198B ->205B 0.13058
198B ->206B 0.14169
199B ->212B 0.19990

Excited State 51: 2.362-A 4.5546 eV 272.22 nm f=0.0425 <S**2>=1.144

193A ->204A -0.13569
197A ->203A 0.43712
198A ->204A 0.28011
199A ->204A 0.17601
200A ->203A 0.26602
168B ->202B -0.10156
171B ->202B -0.13157
175B ->202B -0.16927
186B ->202B 0.11255
188B ->202B -0.26166
190B ->202B -0.10206
195B ->203B -0.14380
198B ->203B 0.49345
199B ->204B -0.22301

Excited State 52: 3.068-A 4.5677 eV 271.43 nm $f=0.0000$ $\langle S^{*2} \rangle=2.104$

198A ->203A	-0.15661
199A ->203A	0.10356
193B ->203B	0.28038
195B ->204B	-0.12019
197B ->203B	-0.20131
198B ->204B	0.62496
199B ->203B	-0.53764

Excited State 53: 2.804-A 4.5747 eV 271.02 nm $f=0.0057$ $\langle S^{*2} \rangle=1.715$

197A ->203A	0.13969
198A ->204A	0.48637
198A ->205A	0.12051
199A ->204A	0.14044
188B ->202B	-0.10346
193B ->204B	-0.27501
195B ->203B	0.13199
196B ->204B	0.13791
197B ->204B	0.16178
197B ->205B	-0.10155
198B ->203B	-0.47198
199B ->204B	0.48338

Excited State 54: 2.234-A 4.6045 eV 269.27 nm $f=0.0004$ $\langle S^{*2} \rangle=0.998$

195A ->204A	-0.23603
196A ->203A	-0.17490
197A ->204A	-0.11101
198A ->203A	0.67395
193B ->203B	0.13389
195B ->204B	-0.18202
196B ->203B	-0.29673
197B ->203B	0.43763
198B ->204B	0.14313

Excited State 55: 3.177-A 4.6180 eV 268.48 nm $f=0.0107$ $\langle S^{*2} \rangle=2.273$

193A ->204A	0.12032
195A ->203A	-0.24279
197A ->203A	-0.23436
198A ->204A	0.65843
188B ->202B	0.27870
194B ->203B	0.13430
197B ->204B	-0.31310

199B ->204B -0.21895

Excited State 56: 2.626-A 4.6325 eV 267.64 nm f=0.0127 <S**2>=1.473

197A ->203A -0.23297

198A ->204A 0.23717

200A ->203A -0.14172

188B ->202B 0.19891

193B ->204B 0.15055

194B ->203B -0.10484

195B ->203B -0.18579

196B ->204B -0.26686

197B ->204B 0.74903

Excited State 57: 2.352-A 4.6328 eV 267.62 nm f=0.0005 <S**2>=1.133

196A ->203A 0.14633

197A ->204A -0.31570

200A ->204A -0.15079

185B ->202B 0.29105

187B ->202B 0.63728

189B ->202B 0.37879

193B ->203B 0.10094

197B ->203B 0.28293

Excited State 58: 3.003-A 4.6374 eV 267.36 nm f=0.0001 <S**2>=2.005

193A ->203A 0.13233

194A ->204A 0.10437

195A ->204A -0.16184

196A ->203A -0.15740

197A ->204A 0.26228

198A ->203A 0.25102

200A ->204A 0.14484

185B ->202B 0.12922

187B ->202B 0.45711

189B ->202B 0.24989

194B ->204B 0.15500

197B ->203B -0.44542

198B ->205B 0.10836

Excited State 59: 2.262-A 4.6380 eV 267.32 nm f=0.0021 <S**2>=1.029

196A ->204A -0.18237

197A ->203A 0.37030

198A ->204A -0.15726

200A ->203A	0.14370
183B ->202B	0.10758
186B ->202B	0.21560
188B ->202B	0.77023
190B ->202B	0.13845
193B ->204B	-0.11236
195B ->203B	-0.13373

Excited State 60: 2.649-A 4.6471 eV 266.80 nm f=0.0003 <S**2>=1.504

194A ->204A	-0.12256
196A ->203A	-0.28725
197A ->204A	0.48702
198A ->203A	-0.33815
200A ->204A	0.15201
201A ->211A	-0.11489
187B ->202B	0.21024
189B ->202B	0.10835
193B ->203B	-0.11355
195B ->204B	-0.32106
196B ->203B	-0.25771
197B ->203B	0.26681
198B ->204B	0.11682
201B ->210B	-0.11710

Excited State 61: 2.683-A 4.7225 eV 262.54 nm f=0.0879 <S**2>=1.550

193A ->204A	0.30510
196A ->204A	-0.26928
197A ->203A	0.27602
202A ->206A	0.13065
202A ->214A	-0.10199
168B ->202B	0.11078
171B ->202B	0.14915
175B ->202B	0.19995
183B ->202B	-0.13699
186B ->202B	-0.28316
188B ->202B	-0.18614
190B ->204B	0.11010
191B ->204B	-0.11301
193B ->202B	-0.10535
193B ->204B	0.23987
196B ->204B	-0.19628
197B ->204B	0.23547

198B ->203B	-0.19903
199B ->204B	-0.17220
201B ->206B	0.13911
201B ->215B	0.11147

Excited State 62: 2.971-A 4.7469 eV 261.19 nm f=0.0000 <S**2>=1.957

191A ->203A	0.10540
193A ->203A	0.23147
194A ->204A	0.11136
195A ->204A	0.17161
197A ->204A	0.10401
200A ->204A	0.10948
200A ->206A	0.10410
201A ->206A	0.11464
201A ->214A	-0.11509
202A ->215A	0.10756
185B ->204B	-0.11759
190B ->203B	0.12491
191B ->203B	-0.12895
193B ->203B	0.46832
194B ->204B	-0.12752
195B ->204B	0.26168
197B ->203B	0.30658
198B ->204B	-0.22902
198B ->206B	0.11067
199B ->203B	-0.23138
201B ->210B	0.10345

Excited State 63: 2.573-A 4.7568 eV 260.64 nm f=0.0821 <S**2>=1.405

195A ->203A	0.26349
196A ->204A	0.20981
197A ->203A	-0.11061
200A ->203A	0.10160
171B ->202B	-0.20420
175B ->202B	-0.18766
180B ->202B	0.13028
186B ->202B	0.28593
188B ->202B	0.11629
193B ->204B	0.38105
195B ->203B	0.38178
196B ->204B	0.13303
197B ->204B	0.21346

198B ->203B	-0.10182
199B ->204B	-0.13836
201B ->206B	0.21235

Excited State 64: 2.694-A 4.7973 eV 258.44 nm f=0.0014 <S**2>=1.565

193A ->204A	0.12806
194A ->203A	-0.43064
195A ->203A	0.74001
196A ->204A	-0.17890
198A ->204A	0.16354
198A ->205A	0.10171
199A ->206A	-0.14229
194B ->203B	0.15608
201B ->206B	-0.11204

Excited State 65: 2.903-A 4.8094 eV 257.80 nm f=0.0002 <S**2>=1.857

194A ->204A	-0.42116
195A ->204A	0.79956
196A ->203A	-0.18074
197A ->206A	-0.10227
198A ->203A	0.16187

Excited State 66: 2.968-A 4.8150 eV 257.49 nm f=0.0003 <S**2>=1.952

199A ->206A	0.10068
194B ->203B	0.72681
195B ->203B	0.44711
196B ->204B	-0.13990
197B ->205B	0.13789
198B ->209B	0.13071
199B ->206B	0.17035
201B ->205B	-0.11409

Excited State 67: 2.763-A 4.8373 eV 256.31 nm f=0.0003 <S**2>=1.659

194B ->204B	0.73975
195B ->204B	0.54166
196B ->203B	-0.19898
198B ->206B	0.10518

Excited State 68: 2.170-A 4.8433 eV 255.99 nm f=0.1016 <S**2>=0.927

193A ->204A	-0.11099
168B ->202B	-0.17508
171B ->202B	0.25002

180B ->202B	-0.34769
183B ->202B	0.73535
186B ->202B	-0.15919
193B ->204B	0.10359
194B ->203B	-0.14478
201B ->205B	0.11200

Excited State 69: 3.264-A 4.8709 eV 254.54 nm f=0.0110 <S**2>=2.413

191A ->204A	-0.10278
193A ->204A	-0.22092
194A ->203A	-0.23989
201A ->215A	0.24376
202A ->205A	-0.10019
202A ->206A	0.22643
202A ->214A	-0.21628
195B ->203B	-0.16154
200B ->214B	-0.25004
201B ->205B	0.16384
201B ->206B	0.50497
201B ->215B	0.23947
201B ->217B	-0.10567

Excited State 70: 3.237-A 4.8848 eV 253.82 nm f=0.0004 <S**2>=2.369

193A ->203A	-0.20896
194A ->204A	-0.27832
196A ->203A	0.19955
196A ->209A	-0.11254
201A ->205A	-0.16801
201A ->206A	0.30692
201A ->214A	-0.26600
201A ->217A	0.15044
202A ->215A	0.31631
181B ->202B	0.11143
184B ->202B	-0.13413
200B ->206B	-0.13460
200B ->213B	0.10829
200B ->215B	-0.19925
200B ->217B	0.14392
201B ->214B	0.31367

Excited State 71: 2.759-A 4.9025 eV 252.90 nm f=0.0020 <S**2>=1.653

193A ->203A	-0.10510
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202A ->216A	0.10011
166B ->202B	0.13077
176B ->202B	0.12292
181B ->202B	0.25412
182B ->202B	0.19086
184B ->202B	-0.32154
185B ->202B	-0.11575
193B ->203B	0.26601
194B ->204B	0.36548
195B ->204B	-0.32870
196B ->203B	0.49012
198B ->204B	-0.10005

Excited State 72: 3.390-A 4.9030 eV 252.87 nm f=0.0029 <S**2>=2.624

194A ->203A	0.38340
194A ->207A	-0.10155
195A ->203A	0.16383
196A ->204A	-0.26947
196A ->208A	-0.13379
197A ->203A	-0.11473
201A ->216A	-0.18159
202A ->213A	0.13796
202A ->217A	0.15787
193B ->204B	0.20527
194B ->203B	0.21196
195B ->203B	-0.25505
195B ->207B	0.13237
196B ->204B	0.35244
196B ->208B	0.14163
200B ->216B	-0.16430
201B ->206B	-0.18328
201B ->213B	-0.15975
201B ->217B	-0.15139

SavETr: write IOETrn= 770 NScale= 10 NData= 16 NLR=1 NState= 72 LETran= 1306.